



chain nodes :

16 17 18 19 20 21 22 23 39 40 41 42 43 44 45 46 47 48 49

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 24 25 26 27 28 29 30 31 32 33 34  
35 36 37 38

chain bonds :

2-22 3-21 4-20 9-16 14-23 16-17 17-18 17-19 25-45 26-44 27-43 32-39 37-46 39-40  
40-41 40-42 46-47 46-48 47-49

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6 5-7 6-11 7-8 7-12 8-9 8-15 9-10 10-11 12-13 13-14 14-15  
24-25 24-29 25-26 26-27 27-28 28-29 28-30 29-34 30-31 30-35 31-32 31-38 32-33  
33-34 35-36 36-37 37-38

exact/norm bonds :

9-16 14-23 16-17 17-19 32-39 39-40 40-42 46-47 46-48 47-49

exact bonds :

2-22 3-21 4-20 5-7 6-11 8-9 9-10 10-11 17-18 25-45 26-44 27-43 28-30 29-34 31-32  
32-33 33-34 37-46 40-41

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-15 12-13 13-14 14-15 24-25 24-29 25-26 26-27  
27-28 28-29 30-31 30-35 31-38 35-36 36-37 37-38

isolated ring systems :

containing 1 : 24 :

G1:H, Ph, Cb, Ak

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 13:Atom 14:Atom 15:Atom 16:CLASS 17:CLASS 18:CLASS 19:CLASS 20:CLASS 21:CLASS  
22:CLASS 23:CLASS 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom  
32:Atom 33:Atom 34:Atom 35:Atom 36:Atom 37:Atom 38:Atom 39:CLASS 40:CLASS 41:CLASS  
42:CLASS 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS

fragments assigned product role:

containing 1

fragments assigned reactant/reagent role:

